



LA-SiGMA

Louisiana Alliance for Simulation-Guided Materials Applications

Louisiana Alliance for Simulation-Guided Materials Applications (LA-SiGMA)

An alliance for transformative and sustainable change in computational materials research, education, outreach, and industrial partnerships throughout the State of Louisiana.



The Materials Genome Initiative launched by the White House in 2011 articulates "a vision of how the development of advanced materials can be accelerated through advances in computational techniques, more effective use of standards, and enhanced data management." LA-SiGMA was formed in 2010 with a very similar vision. LA-SiGMA members are Grambling State University, Louisiana State University, Louisiana Tech University, Southern University at Baton Rouge, Tulane University, University of New Orleans, and Xavier University.

The Alliance pushes the scientific frontiers in computational materials science, and

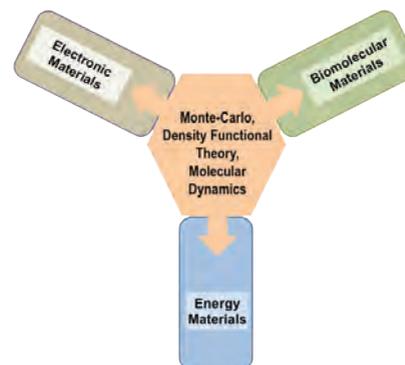
prepares Louisiana researchers to use the next generation of heterogeneous, multicore and hyper-parallel cyberinfrastructure effectively. LA-SiGMA builds statewide interdisciplinary research collaborations involving computational scientists, computer scientists and engineers, applied mathematicians, theorists and experimentalists. Most significantly, the Alliance builds materials science graduate curricula that are unique in its statewide reach and impact, and will be a model for virtual organizations for advanced education and training of graduate students and post-doctoral fellows.

The LA-SiGMA research program consists of three major science drivers in areas of current strength in the State, and of great technological and economic importance:

- (1) **Electronic Materials** - development of multiscale methods for strongly correlated electronic and magnetic systems; studies of correlated organic, ferroelectric, and superconducting materials.
- (2) **Energy Materials** - study of electrochemical cells and capacitors that store and deliver electrical energy, advanced materials for highly efficient and long-lasting batteries and catalytic reactions for fuel generation.
- (3) **Biomolecular Materials** - development of novel biomolecular material systems for the encapsulation, delivery, and release of therapeutics to targeted tissues.

The "glue" that holds the three areas together are the formalisms, algorithms, and codes for tackling multiple length and

time scales and multiscale interactions and correlations. Among these are the next generation Monte Carlo methods, massively parallel implementations of Density Functional Theory, force field methods, and large-scale molecular dynamics.



LA-SiGMA boosts workforce development in the State by creating a multi-tiered set of educational programs, contributing to a well-trained and technologically proficient workforce. The following are the external engagement and workforce development focus areas:

- Middle and high school students are exposed to computational and experimental materials science projects through campus open house events held once per year at all participating institutions.
 - Grades 6-12 and two-year college teachers are part of a summer Research Experiences for Teachers (RET) programs held each summer in New Orleans, Baton Rouge, and Ruston. The Alliance supports 19 RET teachers each summer at different member sites for a six-week program.
 - Multiple programs serve two-year college students. The Alliance is developing short courses to
- provide professional development opportunities for two year college faculty and students. The courses will focus on materials science topics relevant for two-year college curricula and will typically involve hands-on components.
 - Undergraduates at four- and two-year institutions participate in summer research experiences for undergraduates (REU) programs focused on computational and experimental materials science at all LA-SiGMA institutions. The Alliance provides competitive stipends and campus housing for REU students.
 - Graduate students join a transformative educational experience in materials science. A core set of graduate level courses in computational science, multiscale modeling methods, advanced experimental techniques, and other topics are developed and broadcast throughout the State using synchronous HD video. These courses are being integrated into existing and new graduate curricula on each campus.
 - Postdocs and graduate students also participate in a unique program in the use of best practice teaching methods. Undergraduates, graduate students, and postdocs take part in national labs and industrial internships.
 - LA-SiGMA's efforts to increase the participation of women and under-represented minorities in Science, Technology, Engineering and Mathematics are guided by a Diversity Advisory Council made up of national leaders in gender and minority issues in higher education.

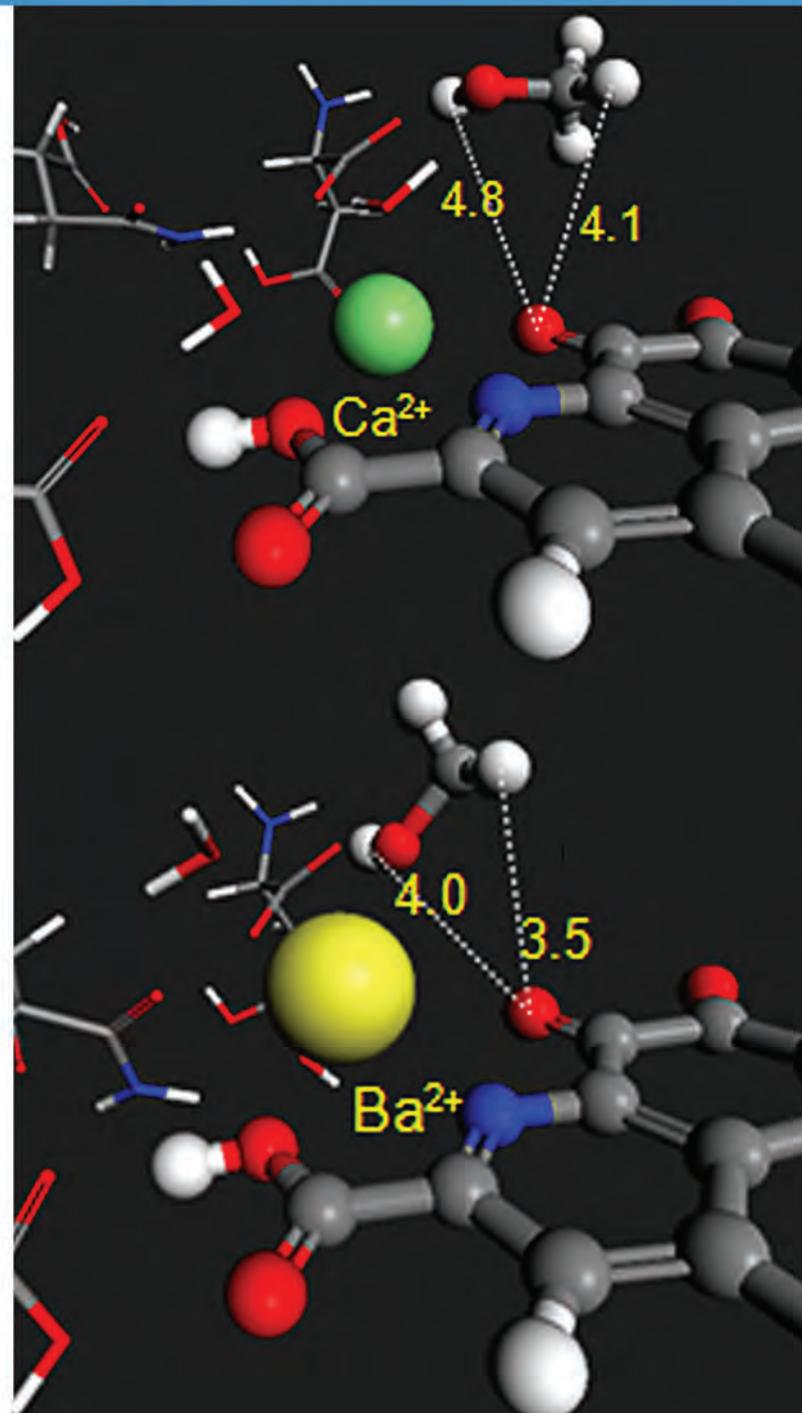
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